09/181,108

(FILE 'HOME' ENTERED AT 13:43:05 ON 12 JUL 2000)

FILE 'REGISTRY' ENTERED AT 13:44:01 ON 12 JUL 2000

L1 STRUCTURE UPLOADED
L2 QUE L1
L3 3 S L2 SSS FULL

FILE 'CAPLUS' ENTERED AT 13:46:24 ON 12 JUL 2000

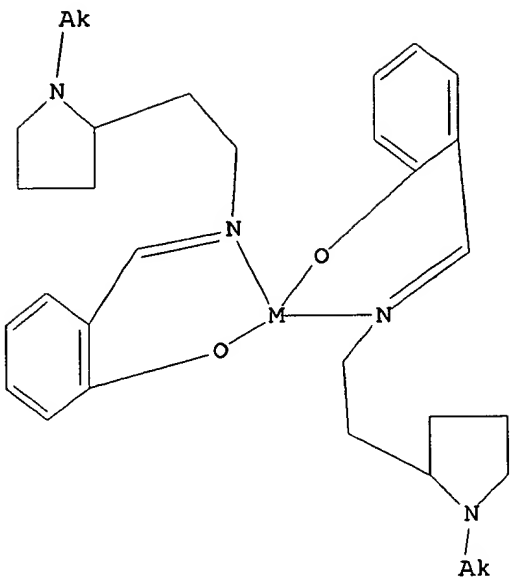
L4 1 S L3

FILE 'CAPLUS, EMBASE, BIOSIS, MEDLINE, WPIDS' ENTERED AT 13:47:32 ON 12 JUL 2000

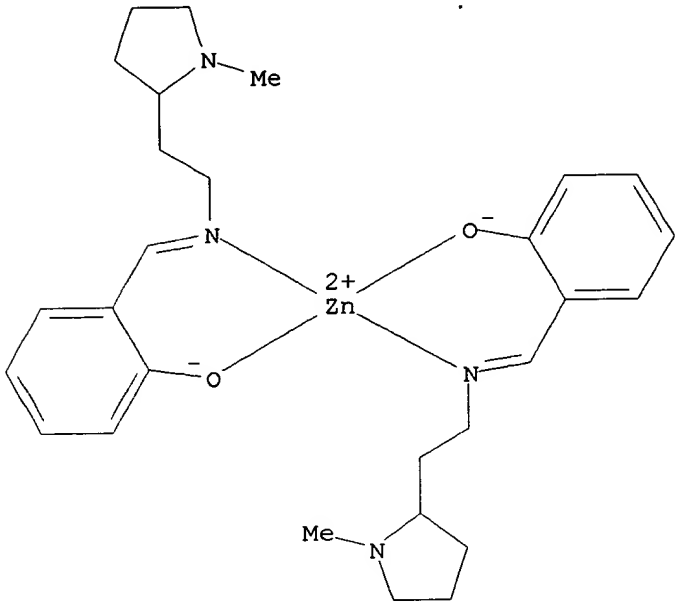
L5 15 S (KLEKOTA, B? OR KLEKOTA B ?)/AU,IN
L6 57 S (MILLER, BENJAMIN ? OR MILLER BENJAMIN ?)/AU,IN
L7 926 S (HAMMOND, M ? OR HAMMOND M ?)/AU,IN
L8 0 S L5 AND L6 AND L7
L9 987 S L5 OR L6 OR L7
L10 18 S L9 AND (COMBINATOR? OR LIBRAR?)
L11 11 DUP REM L10 (7 DUPLICATES REMOVED)
L12 2480 S (BIS)(2A)(SALICYL?)
L13 1815 S L12 AND COMPLEX?
L14 3 S L13 AND (COMBINATOR? OR LIBRAR?)
L15 1 DUP REM L14 (2 DUPLICATES REMOVED)
L16 21628 S (SELF)(2A)(ASSEMBL?)
L17 983 S L16 AND (ZN OR ZINC OR CD OR CADMIUM?)
L18 10 S L17 AND (COMBINATOR? OR LIBRAR?)
L19 6 DUP REM L18 (4 DUPLICATES REMOVED)
L20 84 S (ZINC)(2A)(FINGER?)(3A)(COMBINATOR? OR LIBRAR?)
L21 8 S L20 AND COMPLEX?
L22 0 S L20 AND L16
L23 3 S L12 AND (COMBINAT?)(3A)(LIBRAR?)
L24 22982 S (COORDINAT?)(3A)(COMPLEX?)
L25 762322 S (TRANSITION METAL?) OR ZN OR ZINC
L26 2750 S L24 AND (TRANSITION METAL?)
L27 1817 S L24 AND (ZN OR ZINC)
L28 4004 S L26 OR L27
L29 41 S L28 (L) (COMBINATOR? OR LIBRAR? OR MIXTURE?)
L30 38 DUP REM L29 (3 DUPLICATES REMOVED)
L31 3 S L29 AND (SELF)(2A)(ASSEMB?)
L32 16 S L29 AND (LIGAND? OR RECEPTOR? OR THERAPEUTIC? OR DRUG?)
L33 14 DUP REM L32 (2 DUPLICATES REMOVED)
L34 25 S L29 NOT L32
L35 24 DUP REM L34 (1 DUPLICATE REMOVED)

L2 HAS NO ANSWERS

L1 STR

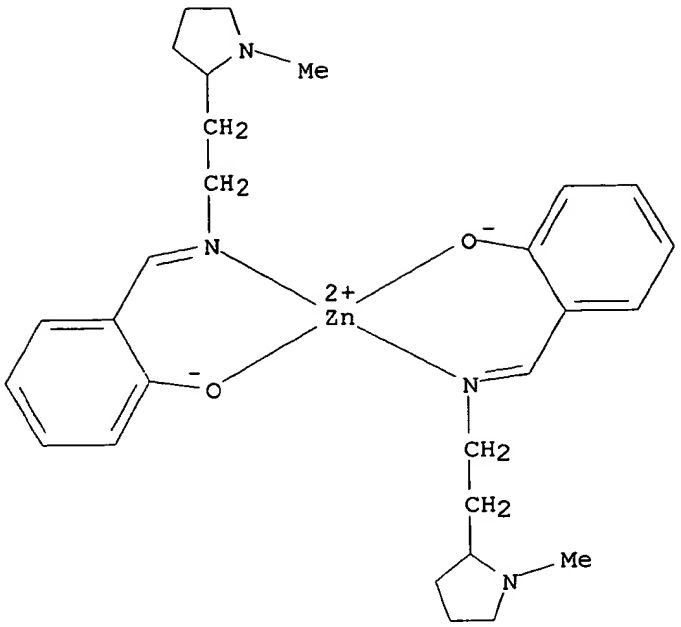


L3 ANSWER 1 OF 3 REGISTRY COPYRIGHT 2000 ACS
RN 202074-94-0 REGISTRY
CN Zinc, bis[2-[[[2-(1-methyl-2-pyrrolidinyl)ethyl]imino-.kappa.N]methyl]phenolato-.kappa.O]-, [T-4-(S),(S)]- (9CI) (CA INDEX NAME)
MF C28 H38 N4 O2 Zn
CI CCS
SR CA
LC STN Files: CA, CAPLUS



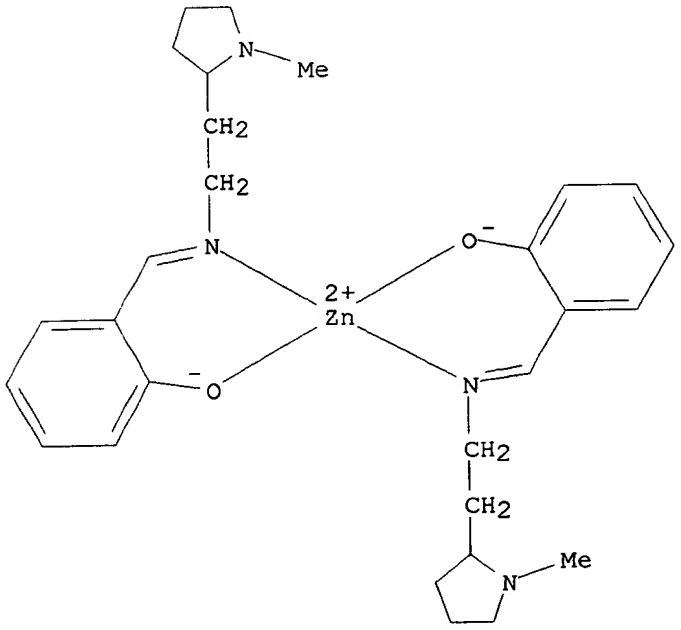
1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

L3 ANSWER 2 OF 3 REGISTRY COPYRIGHT 2000 ACS
RN 202074-93-9 REGISTRY
CN Zinc, bis[2-[[[2-(1-methyl-2-pyrrolidinyl)ethyl]imino-.kappa.N]methyl]phenolato-.kappa.O]-, [T-4-(R),(S)]- (9CI) (CA INDEX NAME)
MF C28 H38 N4 O2 Zn
CI CCS
SR CA
LC STN Files: CA, CAPLUS



1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

L3 ANSWER 3 OF 3 REGISTRY COPYRIGHT 2000 ACS
RN 201986-32-5 REGISTRY
CN Zinc, bis[2-[[[2-(1-methyl-2-pyrrolidinyl)ethyl]imino-.kappa.N]methyl]phenolato-.kappa.O]-, [T-4-(R),(R)]- (9CI) (CA INDEX NAME)
MF C28 H38 N4 O2 Zn
CI CCS
SR CA
LC STN Files: CA, CAPLUS



1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

L4 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2000 ACS

1997:790866 Document No. 128:137688 Generation of novel DNA-binding compounds by selection and amplification from self-assembled combinatorial libraries. Klekota, Bryan; Hammond, Mark H.; Miller, Benjamin L. (Department of Chemistry, University of Rochester, Rochester, NY, 14627, USA). Tetrahedron Lett., 38(50), 8639-8642 (English) 1997. CODEN: TELEAY. ISSN: 0040-4039. Publisher: Elsevier Science Ltd..

AB We describe a general method for the selection of compds. from self-assembled libraries which employs an immobilized receptor (i.e., an affinity reagent) to effect the selection. Using com. available oligo d(A.cntdot.T) DNA-cellulose resin, a set of three stereoisomeric coordination complexes are identified as DNA binding compds. from an equilibrating, self-assembled library of 36 bis(salicylaldiminato)-zinc coordination complexes.

IT **201986-32-5P 202074-93-9P 202074-94-0P**
RL: BPR (Biological process); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC (Process)
(generation of novel DNA-binding compds. by selection and amplification from self-assembled combinatorial libraries)

L11 ANSWER 1 OF 11 CAPLUS COPYRIGHT 2000 ACS
2000:129017 Document No. 133:26372 Dynamic diversity in drug discovery: putting small-molecule evolution to work. Karan, Charles; **Miller, Benjamin L.** (Department of Chemistry, University of Rochester, Rochester, NY, 14627, USA). Drug Discovery Today, 5(2), 67-75 (English) 2000. CODEN: DDTOFS. ISSN: 1359-6446. Publisher: Elsevier Science Ltd..
AB A review with 42 refs. From oligonucleotides to orangutans, nature has found Darwinian evolution to be the most efficient means of optimizing populations of organisms - or mols. Recently, several research groups have begun adapting Darwinian evolution to the identification of small mols. with specific properties. Although still at an early stage, this new field of "dynamic diversity" shows promise as a method for the identification of high-affinity ligands for biomols.

L11 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2000 ACS DUPLICATE 1
1999:625541 Document No. 131:333540 Selection of DNA-binding compounds via multistage molecular evolution. **Klekota, Bryan; Miller, Benjamin L.** (Department of Chemistry, University of Rochester, Rochester, NY, 14627, USA). Tetrahedron, 55(39), 11687-11697 (English) 1999. CODEN: TETRAB. ISSN: 0040-4020. Publisher: Elsevier Science Ltd..
AB **Combinatorial libraries** incorporating multiple equil. offer opportunities to study mol. evolution, and are a novel method of identifying ligands for biol. receptors. We describe the construction and evaluation of a multi-equil. **combinatorial library**, in which structural diversity and structural mutation are accomplished via reversible imine formation and transition-metal complexation. We demonstrate that oligo d(A.cntdot.T)-cellulose resin can select subsets of this **library**, in accord with measured soln.-phase affinities.

L11 ANSWER 3 OF 11 CAPLUS COPYRIGHT 2000 ACS DUPLICATE 2
1999:526036 Document No. 131:266426 Dynamic diversity and small-molecule evolution: a new paradigm for ligand identification. **Klekota, Bryan; Miller, Benjamin L.** (Department of Chemistry, University of Rochester, Rochester, NY, 14627, USA). Trends Biotechnol., 17(5), 205-209 (English) 1999. CODEN: TRBIDM. ISSN: 0167-7799. Publisher: Elsevier Science Ltd..
AB A review with 21 refs. A longstanding goal of org., medicinal and bioorg. chemists has been the discovery of efficient methods for designing or identifying biol. active compds. Recently, several groups have reported using the directed evolution of **combinatorial libraries** as a new method of identifying compds. capable of binding tightly to a target mol. Although significant development remains to be done, the initial results suggest that dynamic diversity and assocd. selection methods will prove to be valuable addns. to the drug-discovery process.

L11 ANSWER 4 OF 11 EMBASE COPYRIGHT 2000 ELSEVIER SCI. B.V.
1999259604 EMBASE Dynamic diversity and small-molecule evolution: A new paradigm for ligand identification. **Klekota B.**; Miller B.L.. B. Klekota, Department of Chemistry, University of Rochester, Rochester, NY 14627, United States. klekota@miller1.chem.rochester.edu. Trends in Biotechnology 17/3 (205-209) 1999.
Refs: 21.
ISSN: 0167-7799. CODEN: TRBIDM.

Publisher Ident.: S 0167-7799(99)01305-0. Pub. Country: United Kingdom. Language: English. Summary Language: English.

AB A longstanding goal of organic, medicinal and bioorganic chemists has been the discovery of efficient methods for designing or identifying biologically active compounds. Recently, several groups have reported using the directed evolution of **combinatorial libraries** as a new method of identifying compounds capable of binding tightly to a target molecule. Although significant development remains to be done, the initial results suggest that dynamic diversity and associated selection methods will prove to be valuable additions to the drug-discovery process.

L11 ~~ANSWER 5 OF 11~~ CAPLUS COPYRIGHT 2000 ACS

1999:145606 Evolving **combinatorial libraries** as a novel method for ligand identification: Pd .pi.-allyl chemistry as a "mutation mechanism". **Klekota, Bryan; Miller, Benjamin L.** (Department of Chemistry, University of Rochester, Rochester, NY, 14627, USA). Book of Abstracts, 217th ACS National Meeting, Anaheim, Calif., March 21-25, ORGN-173. American Chemical Society: Washington, D. C. (English) 1999. CODEN: 67GHA6.

AB **Libraries** generated under equilibrating conditions in the presence of a receptor show promise as a new means of ligand identification. We will describe the results of a **library** selection and amplification scheme in which the Pd-catalyzed transesterification of cyclopentene 1,4 diacetate is used, under equilibrating conditions, to generate ligands for trypsin and thrombin. [Equation Omitted].

L11 ~~ANSWER 6 OF 11~~ BIOSIS COPYRIGHT 2000 BIOSIS

1999:166007 Document No.: PREV199900166007. Evolving **combinatorial libraries** as a novel method for ligand identification: Pd pi-allyl chemistry as a "mutation mechanism. **Klekota, Bryan; Miller, Benjamin L.**. Dep. Chem., Univ. Rochester, Rochester, NY 14627 USA. Abstracts of Papers American Chemical Society, (1999) Vol. 217, No. 1-2, pp. ORGN 173. Meeting Info.: 217th National Meeting of the American Chemical Society Anaheim, California, USA March 21-25, 1999 American Chemical Society. ISSN: 0065-7727. Language: English.

L11 ANSWER 7 OF 11 CAPLUS COPYRIGHT 2000 ACS DUPLICATE 3

1997:790866 Document No. 128:137688 Generation of novel DNA-binding compounds by selection and amplification from self-assembled **combinatorial libraries**. **Klekota, Bryan;** Hammond, Mark H.; **Miller, Benjamin L.** (Department of Chemistry, University of Rochester, Rochester, NY, 14627, USA). Tetrahedron Lett., 38(50), 8639-8642 (English) 1997. CODEN: TELEAY. ISSN: 0040-4039. Publisher: Elsevier Science Ltd..

AB We describe a general method for the selection of compds. from self-assembled **libraries** which employs an immobilized receptor (i.e., an affinity reagent) to effect the selection. Using com. available oligo d(A.cntdot.T) DNA-cellulose resin, a set of three stereoisomeric coordination complexes are identified as DNA binding compds. from an equilibrating, self-assembled **library** of 36 bis(salicylaldiminato)-zinc coordination complexes.

L11 ANSWER 8 OF 11 CAPLUS COPYRIGHT 2000 ACS

1997:162835 Self-assembled, self-amplifying **combinatorial libraries** as a new method for ligand discovery: Application to DNA-binding compounds.. **Klekota, Bryan;** Hammond, Mark H.; **Miller, Benjamin L.** (Department Chemistry, University Rochester, Rochester, NY, 14607, USA). Book of Abstracts, 213th ACS National Meeting, San Francisco, April 13-17, ORGN-573. American Chemical Society: Washington, D. C. (English) 1997. CODEN: 64AOAA.

AB Processes such as the polymerase chain reaction and in vitro selection of

RNA aptamers have demonstrated the power of selection and amplification methods for the identification of biopolymeric ligands to receptors. As part of an effort to study analogous selection and amplification processes for nonbiopolymeric materials, we have developed a self-assembled **combinatorial library** approach to ligand synthesis that employs a solid-supported affinity reagent to select tight-binding compds. from an equilibrating mixt. of coordination compds. Results of the application of this method to the identification of novel DNA-binding compds. will be presented.

L11 ANSWER 9 OF 11 BIOSIS COPYRIGHT 2000 BIOSIS

1997:198282 Document No.: PREV199799497485. Self-assembled, self-amplifying **combinatorial libraries** as a new method for ligand discovery: Application to DNA-binding compounds. **Klekota, Bryan;** Hammond, Mark H.; **Miller, Benjamin L.**. Dep. Chem., Univ. Rochester, Rochester, NY 14607 USA. Abstracts of Papers American Chemical Society, (1997) Vol. 213, No. 1-3, pp. ORGN 573. Meeting Info.: 213th National Meeting of the American Chemical Society San Francisco, California, USA April 13-17, 1997 ISSN: 0065-7727. Language: English.

L11 ANSWER 10 OF 11 CAPLUS COPYRIGHT 2000 ACS

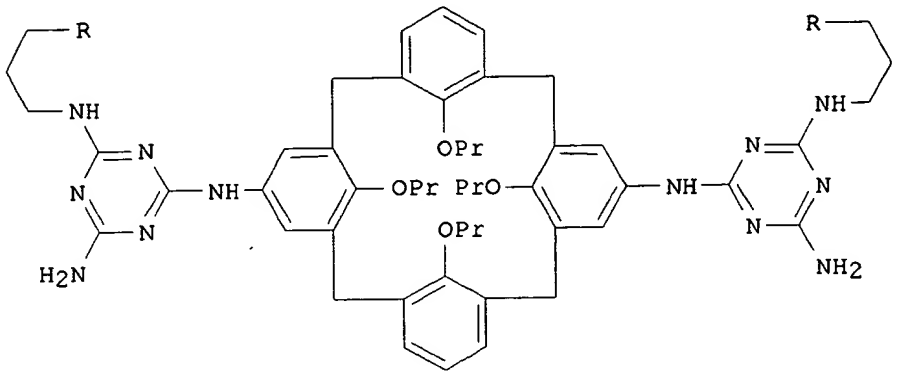
1995:925025 An approach to the discovery of novel ligands for proteins involved in signal transduction. Combs, Andrew P.; Kapoor, Tarun M.; Chen, James K.; **Miller, Benjamin L.**; Miyake, Hiroshi; Feng, Sibo; Yu, Hongtao; Snow, Lygia F.; Gelman, Michael A.; Schreiber, Stuart L. (HHMI, Harvard University, Cambridge, MA, 02138, USA). Book of Abstracts, 210th ACS National Meeting, Chicago, IL, August 20-24, Issue Pt. 2, ORGN-411. American Chemical Society: Washington, D. C. (English) 1995. CODEN: 61XGAC.

AB We screened a biased **combinatorial** peptide **library** and identified unique proline-rich peptides that bind SH3 domains of various signaling proteins. Multidimensional NMR anal. of these receptor-ligand complexes revealed two unique binding modes for the .alpha.-helical peptides to the SH3 domains. Extension of these studies to the discovery of novel non-peptidic ligands via computer modeling, encoded **combinatorial** synthesis and enzymic on-bead assays will be discussed. These studies highlight our four stage approach to ligand discovery: 1) **combinatorial** peptide **library** screening 2) identification of ligands and multidimensional NMR anal. of receptor-ligand complexes, 3) computer modeling directed toward novel **library** design, 4) **combinatorial** synthesis of non-peptidic **libraries** and iteration of steps 2 and 3.

L11 ANSWER 11 OF 11 BIOSIS COPYRIGHT 2000 BIOSIS

1995:422915 Document No.: PREV199598437215. An approach to the discovery of novel ligands for proteins involved in signal transduction. Combs, Andrew P.; Kapoor, Tarun M.; Chen, James K.; **Miller, Benjamin L.**; Miyake, Hiroshi; Feng, Sibo; Yu, Hongtao; Snow, Lygia F.; Gelman, Michael A.; Schreiber, Stuart L.. HHMI, Dep. Chem., Harvard Univ., Cambridge, MA 02138 USA. Abstracts of Papers American Chemical Society, (1995) Vol. 210, No. 1-2, pp. ORGN 411. Meeting Info.: 210th American Chemical Society National Meeting Chicago, Illinois, USA August 20-24, 1995 ISSN: 0065-7727. Language: English.

L19 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2000 ACS
2000:145769 Document No. 132:273224 Guest-templated selection and amplification of a receptor by noncovalent **combinatorial** synthesis. Calama, Mercedes Crego; Timmerman, Peter; Reinhoudt, David N. (Laboratory of Supramolecular Chemistry and Technology MESA Research Institute, University of Twente, Enschede, 7500 AE, Neth.). Angew. Chem., Int. Ed., 39(4), 755-758 (English) 2000. CODEN: ACIEF5. ISSN: 1433-7851.
Publisher: Wiley-VCH Verlag GmbH.
GI



I

AB I (R = (5-(aminocarbonyl-4-phenylene)-10,15,20-tri(4-methylphenyl)porphyrinato)**zinc**) (II) was prepd. by the reaction of bis(chlorotriazine) deriv. of the calix[4]arene with 1,3-propanediamine and ZnL (H2L = 5-(4-chlorocarbonylphenyl)-10,15,20-triphenylporphyrin). The addn. of 1,3,5-tris(4-pyridinyl)benzene (Q) to the H-bonded assembly II3.(DEB)6 (DEB = 5,5-diethylbarbituric acid) gave II3.(DEB)6.Q2. The addn. of Q to a dynamic mixt. of the hydrogen bonded assemblies II3-n.IIIn.(DEB)6 (n = 0-3; III = I (R = Me)) shifted the equil. of the mixt. towards the maximized formation of the strongest receptor II3.(DEB)6 with the complete disappearance of the NMR signals for II3-n.IIIn.(DEB)6 (n = 1, 2). Only NMR signals for III3.(DEB)6 and II3.(DEB)6.Q2 were obsd.

L19 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2000 ACS
1999:71371 Document No. 130:190927 An expansible metalla-cryptand as a component of a supramolecular **combinatorial library** formed from di(8-hydroxyquinoline) ligands and gallium(III) or **zinc**(II) ions. Albrecht, Markus; Blau, Oliver; Frohlich, Roland (Institut fur Organische Chemie der Universitat Richard-Willstatter-Allee, Karlsruhe, D-76131, Germany). Chem.--Eur. J., 5(1), 48-56 (English) 1999.
CODEN: CEUJED. ISSN: 0947-6539. Publisher: Wiley-VCH Verlag GmbH.
AB Ethylene-bridged bis(8-hydroxyquinoline) ligands can be synthesized in five-step procedures from the corresponding 8-hydroxyquinolines. X-ray structural anal. shows that 1,2-bis(8-hydroxyquinolin-7-yl)ethane, (1a-H2) in the solid state forms a polymer by H bonding. When the ligands

1a-1c-H2 (1b, 1c = 3-Bun, 3-decyl analogs of 1a) are mixed with Ga(III) ions, a mixt. (supramol. **combinatorial library**) is formed of coordination compds. {(1a-c)3Ga2}n which by addn. of appropriate guests (M+ = Na+, K+, NH4+, Rb+) can be transformed quant. into a defined metalla-cryptate [M.cntnd.{(1a-c)3Ga2}]+. The gallium and corresponding **Zn** cryptates [M'.cntnd.{(1a)3Zn2}]- (M'+ = Li+, Na+, K+) can also be obtained by metal-directed **self-assembly** processes in the presence of templates. 1H NMR studies and the solid-state structures of [K/Na .cntnd.{(1a)3Ga2}]+ show that the metalla-cryptand {(1a)3Ga2} can adjust to the size of the guest present. Thus, proton H(2) of the ligand acts as a 1H NMR spectroscopic probe to predict the size of the cryptate in soln.

L19 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2000 ACS DUPLICATE 1
1997:790866 Document No. 128:137688 Generation of novel DNA-binding compounds by selection and amplification from **self-assembled combinatorial libraries**. Klekota, Bryan; Hammond, Mark H.; Miller, Benjamin L. (Department of Chemistry, University of Rochester, Rochester, NY, 14627, USA). Tetrahedron Lett., 38(50), 8639-8642 (English) 1997. CODEN: TELEAY. ISSN: 0040-4039. Publisher: Elsevier Science Ltd..

AB We describe a general method for the selection of compds. from **self-assembled libraries** which employs an immobilized receptor (i.e., an affinity reagent) to effect the selection. Using com. available oligo d(A.cntdot.T) DNA-cellulose resin, a set of three stereoisomeric coordination complexes are identified as DNA binding compds. from an equilibrating, **self-assembled library** of 36 bis(salicylaldiminato)-**zinc** coordination complexes.

L19 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2000 ACS
1997:166031 Document No. 126:247939 De novo design of heterotrimeric coiled coils. Lombardi, Angela; Bryson, James W.; DeGrado, William F. (Centro Interdipartimentate Ricerca Peptidi Bioattivi, University Napoli "Federico II", Naples, 80134, Italy). Biopolymers, Volume Date 1996, 40(5), 495-504 (English) 1997. CODEN: BIPMAA. ISSN: 0006-3525. Publisher: Wiley.

AB The three-helix bundle is a common structural motif among natural proteins. It has been obsd. in numerous important proteins, such as fibrinogen, laminin, spectrin, dystrophin, hemagglutinin, and mannose binding proteins. The three-helix bundle is a simple structure in which three .alpha.-helix pack against each other, with a slight left-handed twist. Because of its simplicity relative to other structural motifs, the three-helix bundle can be conveniently used both to clarify the forces responsible for the protein folding and stability, and for the design of novel proteins. In this paper we describe the design, synthesis, and characterization of three peptides that **self-assemble** into antiparallel, heterotrimeric coiled coils. The exptl. results, obtained from CD spectroscopy and ultracentrifugation equil. sedimentation, indicate that the mixt. of the three peptides preferentially forms heterotrimers; moreover, these aggregates represent attractive systems for **combinatorial** design of **libraries** of pseudo C3 sym. ligands or binding sites.

L19 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2000 ACS
1996:494554 Document No. 125:236812 Design and Study of Synthetic Chiral Nanoscopic Assemblies. Preparation and Characterization of Optically Active Hybrid, Iodonium-Transition-Metal and All-Transition-Metal Macrocyclic Molecular Squares. Olenyuk, Bogdan; Whiteford, Jeffery A.; Stang, Peter J. (Department of Chemistry, University of Utah, Salt Lake City, UT, 84112, USA). J. Am. Chem. Soc., 118(35), 8221-8230 (English) 1996. CODEN: JACSAT. ISSN: 0002-7863.

AB The synthesis and characterization of various optically active nanoscale-size tetranuclear assemblies held together by coordination bonds is described. Interaction of bis[4-(4'-pyridyl)phenyl]iodonium triflate and bis triflates of chiral transition metal (Pd(II) or Pt(II)) diphosphines gave chiral hybrid iodonium-transition metal mol. squares. Restricted rotation of the coordinated bis[4-(4'-pyridyl)phenyl]iodonium moiety was detected in these squares and studied by using variable-temp. NMR. The prepn. of chiral hybrid squares which possess the elements of helicity (twist) in the assembly was accomplished using the above bisphosphines and bis(3-pyridyl)iodonium triflate. Interaction between the bis triflates of chiral (R(+)-BINAP or S(-)-BINAP) transition metal (Pd(II) or Pt(II)) bisphosphines and a diaza ligand with C2h symmetry, 2,6-diazaanthracene (DAA) or 2,6-diazaanthracene-9,10-dione (DAAD), in acetone at ambient temp. results in chirality-directed assembly of a single stable diastereomer or highly enriched diastereomeric mixts. of optically active macrocyclic mol. squares. The stereochem. outcome of such **self-assembly** at the full **combinatorial** level was studied as well using achiral Pd(II) or Pt(II) bisphosphine complexes.

L19 ANSWER 6 OF 6 EMBASE COPYRIGHT 2000 ELSEVIER SCI. B.V.DUPLICATE 2

97082719 EMBASE Document No.: 1997082719. De novo design of heterotrimeric coiled coils. Lombardi A.; Bryson J.W.; DeGrado W.F.. A. Lombardi, I CIRPB, Ctro. Studio Biocristallog. del CNR, University of Napoli 'Federico II', Via Mezzocannone 4, 80134 Napoli, Italy. Biopolymers - Peptide Science Section 40/5 (495-504) 1996.

Refs: 45.

ISSN: 0006-3525. CODEN: BPSSFT. Pub. Country: United States. Language: English. Summary Language: English.

AB The three-helix bundle is a common structural motif among natural proteins. It has been observed in numerous important proteins, such as fibrinogen, laminin, spectrin, dystrofin, hemagglutinin, and mannose binding proteins. The three-helix bundle is a simple structure in which three .alpha.- helices pack against each other, with a slight left-handed twist. Because of its simplicity relative to other structural motifs, the three-helix bundle can he conveniently used both to clarify the forces responsible for the protein folding and stability, and for the design of novel proteins. In this paper we describe the design, synthesis, and characterization of three peptides that **self-assemble** into antiparallel, heterotrimeric coiled coils. The experimental results, obtained from **CD** spectroscopy and ultracentrifugation equilibrium sedimentation, indicate that the mixture of the three peptides preferentially forms heterotrimers; moreover, these aggregates represent attractive systems for **combinatorial** design of **libraries** of pseudo C3 symmetric ligands or binding sites.

L21 ANSWER 1 OF 8 CAPLUS COPYRIGHT 2000 ACS
1999:548520 Document No. 131:296712 Dimerization of zinc fingers mediated by peptides evolved in vitro from random sequences. Wang, Bryan S.; Pabo, Carl O. (Howard Hughes Medical Institute and Department of Biology, Massachusetts Institute of Technology, Cambridge, MA, 02139, USA). Proc. Natl. Acad. Sci. U. S. A., 96(17), 9568-9573 (English) 1999. CODEN: PNASA6. ISSN: 0027-8424. Publisher: National Academy of Sciences.
AB Peptides that mediate dimerization of attached zinc finger DNA-binding domains have been evolved in vitro starting from random sequences. The authors first used phage display to select dimerization elements from libraries of random 15-residue polypeptides that were fused to the N terminus of the zinc finger domains. The authors then reoptimized these peptides by sequentially randomizing five-residue blocks (proceeding across the peptide in three steps) and selecting variant peptides that further stabilized the protein-DNA **complex**. Biochem. expts. confirmed that the selected peptides promote dimerization of the zinc fingers on an appropriate DNA target site. These results demonstrate that dimerization units can be obtained readily from random polypeptide libraries of moderate **complexity**. Our success reemphasizes the utility of searching random peptide libraries in protein design projects, and the sequences presented here may be useful when designing novel transcription factors.

L21 ANSWER 2 OF 8 CAPLUS COPYRIGHT 2000 ACS
1995:489791 Document No. 123:262 A conformationally homogeneous combinatorial peptide library. Bianchi, Elisabeta; Folgori, Antonella; Wallace, Andrew; Nicotra, Maria; Acali, Stefano; Phalipon, Armelle; Barbato, Gaetano; Bazzo, Renzo; Cortese, Riccardo (Dep. of Biotechnology, Inst. di Richerche di Biologia Molecolare P. Angeletti, Pomezia, 00040, Italy). J. Mol. Biol., 247(2), 154-60 (English) 1995. CODEN: JMOBAK. ISSN: 0022-2836.
AB In search for a rational way to convert the information encoded in peptide structures into peptidomimetics, major progress could be made by coupling the power-of-selection methods, now enormously increased in no. as a result of the development of combinatorial peptide libraries, with the rational design of structure-inducing templates for the selectable sequences. The availability of libraries of peptides with predetd. structure would enable selection-driven peptidomimetic design, whereby a conformational model for the peptide pharmacophore would be directly derived from the screening, allowing the design of a suitable non-peptidic scaffold to replace the peptide backbone. The authors describe here the first example of a conformationally homogeneous combinatorial peptide library, which yields ligands with the expected structure upon selection. The library was built by randomizing five positions in the .alpha.-helical portion of a 26 amino acid Cys2His2 consensus "zinc-finger" motif. Since in zinc-fingers metal coordination and folding are coupled, in the library metal-dependent binding represents a built-in control against the selection of structurally undefined sequences. The .alpha.-helical library was produced as both fusion with the p VIII protein of filamentous phage and sol. peptides by chem. synthesis, the latter enabling the expansion of the selectable repertoire by the inclusion of non-coded amino

acids. The two libraries were independently screened with the same receptor (a monoclonal IgA reactive against the lipopolysaccharide of the human pathogen Shigella flexneri), yielding a very similar consensus. In particular, the peptides defined by both methods showed very strong, zinc-dependent binding to the IgA. The geometrical arrangement of the side-chains of the selected peptide pharmacophore was shown by CD, Co(II)-
complex absorption and high-resoln. NMR to be structurally invariant with respect to the parent zinc-finger.

L21 ANSWER 3 OF 8 CAPLUS COPYRIGHT 2000 ACS
1995:227782 Document No. 122:153180 Differential interaction of the dual .alpha.tropomyosin/N5 enhancer with multiple DNA binding proteins: N5 is a
putative novel Z-ZIP DNA binding protein. Ruiz-Opazo, Nelson; Cloix, Jean-Francois; Herrera, Victoria L. (Whitaker Cadiovascular Institute, Boston University School Medicine, Boston, MA, 02118, USA). Cell. Mol. Biol. Res., 40(4), 265-72 (English) 1994. CODEN: CMBREW. ISSN: 0968-8773.

AB The .alpha. tropomyosin (TM)/N5 enhancer is an SV40-like mammalian enhancer comprised of a 99 bp repeat with modular cis-acting regulatory elements exhibiting apparent hierarchical organization. The enhancer differentially regulates the .alpha.TM and N5 transcription units which exhibit distinct tissue-specific expression patterns and interacts with multiple myotube-assocd. nuclear DNA binding proteins that varied in size and amt. To further characterize the interaction with multiple myotube nuclear factors, comparative southwestern blot analyses were done with a panel of strategic DNA probes representative of modular enhancer sequences
in the .alpha.TM/N5 enhancer and resp. .alpha.TM and N5 promoter regions. Multiple DNA binding proteins, which vary in size and amt., can interact with a particular enhancer modular sequence (delimited to 18 bp- to 38 bp-long); likewise, a DNA binding protein can bind specifically to different DNA enhancer modular sequences with apparent different affinities. DNA binding proteins that differentially bind to both enhancer modular sequences and resp. promoter regions supporting a putative parsimonious mechanism for the approxn. of enhancer and promoter elements as an alternative to the multi-protein stereospecific enhancer **complex**. Cogent to this interesting "head to head"/shared enhancer gene arrangement, we investigated the primary structure of the "other" transcription unit, N5. Nucleotide sequence anal. of the N5 cDNA reveals that is a putative DNA binding protein representing a new structural class of transcription factors exhibiting a novel **combinatorial** motif: single **zinc finger** (DNA-binding)-leucine zipper (dimerization) - making it a z-ZIP instead of
a b-ZIP (basic region/leucine zipper) protein.

L21 ANSWER 4 OF 8 EMBASE COPYRIGHT 2000 ELSEVIER SCI. B.V.
95008659 EMBASE Document No.: 1995008659. Differential interaction of the dual .alpha.tropomyosin/N5 enhancer with multiple DNA binding proteins: N5
is a putative novel z-ZIP DNA binding protein. Ruiz-Opazo N.; Cloix J.-F.;
Herrera V.L.M.. Section of Molecular Genetics, Whitaker Cardiovascular Institute, Boston University School of Medicine, 80 East Concord Street,Boston, MA 02118, United States. Cellular and Molecular Biology Research 40/4 (265-272) 1994.
ISSN: 0968-8773. CODEN: CMBREW. Pub. Country: United Kingdom. Language: English. Summary Language: English.

AB The .alpha. tropomyosin (TM)/N5 enhancer is an SV40-like mammalian enhancer comprised of a 99 bp repeat with modular cis-acting regulatory elements exhibiting apparent hierarchical organization. The enhancer differentially regulates the .alpha.TM and N5 transcription units which exhibit distinct tissue-specific expression patterns and interacts with multiple myotube-associated nuclear DNA binding proteins that varied in

size and amount. To further characterize the interaction with multiple myotube nuclear factors, comparative southwestern blot analyses were done with a panel of strategic DNA probes representative of modular enhancer sequences in the .alpha.TM/N5 enhancer and respective .alpha.TM and N5 promoter regions. Results demonstrate that multiple DNA binding proteins, which vary in size and amount, can interact with a particular enhancer modular sequence (delimited to 18 bp- to 38 bp-long); and that likewise, a DNA binding protein can bind specifically to different DNA enhancer modular sequences with apparent different affinities. Results also demonstrate DNA binding proteins that differentially bind to both enhancer modular sequences and respective promoter regions supporting a putative parsimonious mechanism for the approximation of enhancer and promoter elements as an alternative to the multi-protein stereospecific enhancer **complex**. Cogent to this interesting 'head to head'/shared enhancer gene arrangement, we investigated the primary structure of the 'other' transcription unit, N5. Nucleotide sequence analysis of the N5 cDNA reveals that it is a putative DNA binding protein representing a new structural class of transcription factors exhibiting a novel **combinatorial** motif: single **zinc finger** (DNA-binding)-leucine zipper (dimerization) - making it a z-ZIP instead of a b-ZIP (basic region/leucine zipper) protein.

L21 ANSWER 5 OF 8 EMBASE COPYRIGHT 2000 ELSEVIER SCI. B.V.

94346312 EMBASE Document No.: 1994346312. Selection of DNA binding sites for zinc fingers using rationally randomized DNA reveals coded interactions. Choo Y.; Klug A.. Laboratory of Molecular Biology, Medical Research Council, Hills Road,Cambridge CB2 2QH, United Kingdom. Proceedings of the National Academy of Sciences of the United States of America 91/23 (11168-11172) 1994.
ISSN: 0027-8424. CODEN: PNASA6. Pub. Country: United States. Language: English. Summary Language: English.

AB In the preceding paper [Choo, Y. and Klug, A. (1994) Proc. Natl. Acad. Sci. USA 91, 11163-11167], we showed how selections from a **library** of **zinc fingers** displayed on phage yielded fingers able to bind to a number of DNA triplets. Here, we describe a technique to deal efficiently with the converse problem-namely, the selection of a DNA binding site for a given zinc finger. This is done by screening against libraries of DNA triplet binding sites randomized in two positions but having one base fixed in the third position. The technique is applied here to determine the specificity of fingers previously selected by phage display. We find that some of these fingers are able to specify a unique base in each position of the cognate triplet. This is further illustrated by examples of fingers which can discriminate between closely related triplets as measured by their respective equilibrium dissociation constants. Comparing the amino acid sequences of fingers which specify a particular base in a triplet, we infer that in most instances, sequence-specific binding of zinc fingers to DNA can be achieved by using a small set of amino acid-nucleotide base contacts amenable to a code.

L21 ANSWER 6 OF 8 EMBASE COPYRIGHT 2000 ELSEVIER SCI. B.V.

94346311 EMBASE Document No.: 1994346311. Toward a code for the interactions of zinc fingers with DNA: Selection of randomized fingers displayed on phage. Choo Y.; Klug A.. Medical Research Council, Laboratory of Molecular Biology, Hills Road,Cambridge CB2 2QH, United Kingdom. Proceedings of the National Academy of Sciences of the United States of America 91/23 (11163-11167) 1994.
ISSN: 0027-8424. CODEN: PNASA6. Pub. Country: United States. Language: English. Summary Language: English.

AB We have used two selection techniques to study sequence-specific DNA recognition by the zinc finger, a small, modular DNA-binding minidomain.

We have chosen zinc fingers because they bind as independent modules and so can be linked together in a peptide designed to bind a predetermined DNA site. In this paper, we describe how a **library** of **zinc fingers** displayed on the surface of bacteriophage enables selection of fingers capable of binding to given DNA triplets. The amino acid sequences of selected fingers which bind the same triplet are compared to examine how sequence-specific DNA recognition occurs. Our results can be rationalized in terms of coded interactions between zinc fingers and DNA, involving base contacts from a few .alpha.-helical positions. In the paper following this one, we describe a complementary technique which confirms the identity of amino acids capable of DNA sequence discrimination from these positions.

L21 ANSWER 7 OF 8 BIOSIS COPYRIGHT 2000 BIOSIS

1995:80214 Document No.: PREV199598094514. Differential interaction of the dual alpha-tropomyosin/N5 enhancer with multiple DNA binding proteins: N5 is a putative novel Z-ZIP DNA binding protein. Ruiz-Opazo, Nelson (1); Cloix, Jean-Francois; Herrera, Victoria L. M.. (1) Sect. Molecular Genetics, Whitaker Cardiovascular Inst., Boston Univ. Sch. Med., 80 East Concord St., Boston, MA 02118 USA. Cellular & Molecular Biology Research, (1994) Vol. 40, No. 4, pp. 265-272. Language: English.

AB The alpha tropomyosin (TM)/N5 enhancer is an SV40-like mammalian enhancer comprised of a 99 bp repeat with modular cis-acting regulatory elements exhibiting apparent hierarchical organization. The enhancer differentially regulates the alpha-TM and N5 transcription units which exhibit distinct tissue-specific expression patterns and interacts with multiple myotube-associated nuclear DNA binding proteins that varied in size and amount. To further characterize the interaction with multiple myotube nuclear factors, comparative southwestern blot analyses were done with a panel of strategic DNA probes representative of modular enhancer sequences in the alpha-TM/N5 enhancer and respective alpha-TM and N5 promoter regions. Results demonstrate that multiple DNA binding proteins, which vary in size and amount, can interact with a particular enhancer modular sequence (delimited to 18 bp- to 38 bp-long); and that likewise, a DNA binding protein can bind specifically to different DNA enhancer modular sequences with apparent different affinities. Results also demonstrate DNA binding proteins that differentially bind to both enhancer modular sequences and respective promoter regions supporting a putative parsimonious mechanism for the approximation of enhancer and promoter elements as an alternative to the multi-protein stereospecific enhancer **complex**. Cogent to this interesting "head to head"/shared enhancer gene arrangement, we investigated the primary structure of the "other" transcription unit, N5. Nucleotide sequence analysis of the N5 CDNA reveals that it is a putative DNA binding protein representing a new structural class of transcription factors exhibiting a novel **combinatorial** motif: single **zinc finger** (DNA-binding)-leucine zipper (dimerization) making it a z-ZIP instead of a b-ZIP (basic region/leucine zipper) protein.

L21 ANSWER 8 OF 8 MEDLINE

95170763 Document Number: 95170763. Differential interaction of the dual alpha tropomyosin/N5 enhancer with multiple DNA binding proteins: N5 is a putative novel z-ZIP DNA binding protein. Ruiz-Opazo N; Cloix J F; Herrera V L. (Section of Molecular Genetics, Whitaker Cardiovascular Institute, Boston University School of Medicine, MA 02118..) CELLULAR AND MOLECULAR BIOLOGY RESEARCH, (1994) 40 (4) 265-72. Journal code: BSK. ISSN: 0968-8773. Pub. country: United States. Language: English.

AB The alpha tropomyosin (TM)/N5 enhancer is an SV40-like mammalian enhancer comprised of a 99 bp repeat with modular cis-acting regulatory elements exhibiting apparent hierarchical organization. The enhancer differentially

regulates the alpha TM and N5 transcription units which exhibit distinct tissue-specific expression patterns and interacts with multiple myotube-associated nuclear DNA binding proteins that varied in size and amount. To further characterize the interaction with multiple myotube nuclear factors, comparative southwestern blot analyses were done with a panel of strategic DNA probes representative of modular enhancer sequences in the alpha TM/N5 enhancer and respective alpha TM and N5 promoter regions. Results demonstrate that multiple DNA binding proteins, which vary in size and amount, can interact with a particular enhancer modular sequence (delimited to 18 bp- to 38 bp-long); and that likewise, a DNA binding protein can bind specifically to different DNA enhancer modular sequences with apparent different affinities. Results also demonstrate DNA binding proteins that differentially bind to both enhancer modular sequences and respective promoter regions supporting a putative parsimonious mechanism for the approximation of enhancer and promoter elements as an alternative to the multi-protein stereospecific enhancer **complex**. Cogent to this interesting "head to head"/shared enhancer gene arrangement, we investigated the primary structure of the "other" transcription unit, N5. Nucleotide sequence analysis of the N5 cDNA reveals that it is a putative DNA binding protein representing a new structural class of transcription factors exhibiting a novel **combinatorial** motif: single **zinc finger** (DNA-binding)-leucine zipper (dimerization)--making it a z-ZIP instead of a b-ZIP (basic region/leucine zipper) protein.

L33 ANSWER 1 OF 14 WPIDS COPYRIGHT 2000 DERWENT INFORMATION LTD
AN 2000-037098 [03] WPIDS
AB US 5976887 A UPAB: 20000118
NOVELTY - A reaction **mixture** is formed with a sample suspected of containing a diamino aromatic **ligand**. Subsequently, the **ligand** is induced to produce an electrochemiluminescent (ELC) response thereby indicating it's presence in the sample.

DETAILED DESCRIPTION - INDEPENDENT CLAIM is included for:

(1) electrochemiluminescent complex comprising:

(a) a diamino aromatic **ligand** which is 2,4-diaminotoluene, 3,4- diaminotoluene or 2,3-diaminonaphthalene; and

(b) a soluble metal ion of gold (Au+), chromium (Cr6+), iron (Fe3+), ruthenium (Ru3+) or vanadium (V5+) and is induced to electrochemiluminescence; and

(2) use in detecting the breakdown or byproducts of trinitrotoluene.

USE - For detecting breakdown or byproducts of trinitrotoluene (TNT) (claimed), other nitro aromatics, for detecting toxic metals, soluble metal ions and diamino aromatic **ligands** in industrial waste water streams, soil, ground water, for detecting biotoxins, nucleic acid and bacterial pathogens, for quantifying of **transition metal** ions, for determining atomic or intermolecular distances, for studying electronic states of molecules and characterizing **coordinating** bonding of **complex** exhibiting ECL upon bonding.

ADVANTAGE - ECL assays are extremely sensitive, rapid, simple and inexpensive. Luminescence in ECL can be controlled by an applied voltage at the working electrode.

DESCRIPTION OF DRAWING(S) - The figure is the schematic representation of the ECL assay interaction between the metal ion and the diamino aromatic in solution.

Diaminotoluene-metal ion interaction; I

Diaminonaphthalene- metal ion interaction II

Dwg.13/13

L33 ANSWER 2 OF 14 WPIDS COPYRIGHT 2000 DERWENT INFORMATION LTD
AN 1998-467462 [40] WPIDS
AB WO 9837040 A UPAB: 19981008
A gas generant composition (C) for inflating an automotive airbag passive restraint system comprising: at least one metal **coordination complex** (MC) comprising a **transition metal**, a nitrogen and hydrogen containing **ligand**, and an anionic component to balance the charge of the complex; and at least one high nitrogen fuel (F) selected from the group consisting of non-azide and azide fuels (AF), with the proviso that the gas generant composition does not contain the following: cobalt (III) triammine trinitrate, Co (NH3)3(NO3)3, or; copper (II) diammine dinitrate, Cu(NH3)3 (NO3)3, and an oxide **mixture** of V2O5,MoO3.

USE - Inflation of safety restraints in motor vehicles (airbags)

ADVANTAGE - Non-azide, high density and reduced sensitivity gas generant which produces abundant amounts of water vapour and gas such as CO2, N2 and O2.

Dwg.0/0

L33 ANSWER 3 OF 14 WPIDS COPYRIGHT 2000 DERWENT INFORMATION LTD
AN 1998-427018 [36] WPIDS
AB US 5783378 A UPAB: 19980911
A radiation sensitive emulsion comprises silver halide grains and a gelatino-peptiser for the grains that contains < 30 mu moles of

methionine/g. The silver halide grains contain > 50 mole% chloride based on silver and > 50% of their surface area is provided by (100) crystal faces. A central portion of the grains accounts for 95-98% of total silver and contains 3 dopants: (D1) which is a metal **coordination complex** containing a nitrosyl or thionitrosyl **ligand** in combination with a group 5-10 **transition metal**; (D2) which is a shallow electron trapping dopant; and (D3) which is an iridium **coordination complex** having **ligands** which are more electropositive than cyano.

USE - The emulsion is useful in photography.

ADVANTAGE - The combination of dopants and low methionine gelatino-peptiser provides higher instantaneous contrast over a range of densities and results in colour print images showing increased shadow detail. By placing the dopants within the central portion of the grains, they are protected from competing and/or antagonist effects that can occur at the surface of the grains as a result of chemical and spectral sensitisation and the addition of other adsorbed materials.

Dwg.0/0

L33 ANSWER 4 OF 14 CAPLUS COPYRIGHT 2000 ACS DUPLICATE 1

1997:790866 Document No. 128:137688 Generation of novel DNA-binding compounds by selection and amplification from self-assembled **combinatorial libraries**. Klekota, Bryan; Hammond, Mark H.; Miller, Benjamin L. (Department of Chemistry, University of Rochester, Rochester, NY, 14627, USA). Tetrahedron Lett., 38(50), 8639-8642 (English) 1997. CODEN: TELEAY. ISSN: 0040-4039. Publisher: Elsevier Science Ltd..

AB We describe a general method for the selection of compds. from self-assembled **libraries** which employs an immobilized **receptor** (i.e., an affinity reagent) to effect the selection. Using com. available oligo d(A.cntdot.T) DNA-cellulose resin, a set of three stereoisomeric **coordination complexes** are identified as DNA binding compds. from an equilibrating, self-assembled **library** of 36 bis(salicylaldiminato)-**zinc coordination complexes**.

L33 ANSWER 5 OF 14 CAPLUS COPYRIGHT 2000 ACS

1996:544189 Document No. 125:236878 **Combinatorial** Approach to the Discovery of Novel **Coordination Complexes**. Francis, Matthew B.; Finney, Nathaniel S.; Jacobsen, Eric N. (Department of Chemistry, Harvard University, Cambridge, MA, 02138, USA). J. Am. Chem. Soc., 118(37), 8983-8984 (English) 1996. CODEN: JACSAT. ISSN: 0002-7863.

AB Metal complexes are reported as formed using a **library** from **combinatorial** chem. The **library** was prepd. on poly(ethylene glycol)-grafted polystyrene so that each polymer bead displayed a unique **ligand** structure. The **library** theor. consisted of 12,000 different **ligands**. It comprises 4 variable components: 2 amino acids linked by a "turn element" and terminated by various capping reagents. The turn elements employed were cyclic 1,2-amino alcs. or .alpha.-amino acid derivs. Metals used were Ni, Fe, Cu, Pt, Sn, and Pd. With Ni, 4 different **ligands** were found each bearing L-His(Trt) in both amino acid positions; only 2 turn elements, acetyl and 1-naphthylenyl chlorides, were found. Extent of binding is reported for the other metals with some general observations regarding selectivity of amino acids.

L33 ANSWER 6 OF 14 CAPLUS COPYRIGHT 2000 ACS

1996:414162 **Combinatorial** approaches to the discovery of new **coordination complexes**. Francis, Matthew B.; Finney, Nathaniel S.; Jacobsen, Eric N. (Harvard University, Cambridge, MA, 02138,

USA). Book of Abstracts, 212th ACS National Meeting, Orlando, FL, August 25-29, INOR-005. American Chemical Society: Washington, D. C. (English) 1996. CODEN: 63BFAF.

AB The relationship of **ligand** structure to the chem. and phys. properties of derived metal complexes is a central theme in such vital and disparate fields as selective catalysis, sensor discovery, and bioinorg. chem. The signal advances in these disciplines made over the past several years highlight not only the utility of complexes with well-designed structural, electronic, or stereochem. features, but also the challenges assocd. with such design. Since the stability and properties of metal complexes are dependent on interrelated variables such as the coordination geometry required by the metal and the steric and electronic characteristics of the **ligand**, **combinatorial** chem. could provide a powerful approach for discovering new types of coordination compds. This lecture will outline our preliminary studies in the selective binding of **transition metal** ions by **ligands** prepd. by solid-phase **combinatorial** synthesis.

L33 ANSWER 7 OF 14 WPIDS COPYRIGHT 2000 DERWENT INFORMATION LTD

AN 1993-190159 [24] WPIDS

AB EP 546808 A UPAB: 19931116

Compsn. (I) comprises (A) a hexacoordinate organometallic complex, and (B) a solvent of solubility parameter at least 20 MPa 1/2 (A) consists of a metal (M) selected from Mo, W and Gps. 7, 8 and 9, and at least one **ligand** (L) capable of providing five coordinating atoms to (A). (B) is capable of dissolving (A) to at least 0.1 M.

Pref. (M) is Mo(O), W(O), Re(I), Re(II), Fe(I), Fe(II), Co(O), Co(I), Os(II), Ir(I), Rh(I) or Mn(I). (L) may be monodentate (e.g. halogen, hydride, carbon monoxide, amine or phosphine), bidentate (e.g. phosphine, phosphite, thiol, sulphide or amine), or tridentate, tetradentate or pentadentate (e.g. phosphine or amine). Further **ligand**(s) may be present, e.g. halogen, hydride, nitrogen, carbon monoxide, nitrogen-contg. base, phosphine, pyridine or imidazole.

USE/ADVANTAGE - (I) is of use for selective removal of nitrogen from other gases, esp. from natural gas. The method is simple, efficient and of low cost.

Dwg.0/5

ABEQ US 5225174 A UPAB: 19931116

Sepn. of nitrozen comprises absorbing N2 from a N2-contg. feed stream contg. 01-80 vol% N2 by contacting the feed stream with a compsn. comprising solvent and an organs metallic complex, which consists of a **transition metal** e.g. Mo, W and a metal from gps. 7,8 and 9. and one or more liquids which provide 5 or 6 coordinating atoms to the organometallic complex. The solvent can dissolve the organometallic complex to at least 0.1 M and (6) desorbing N2 from the compsn. to a prod. stream.

USE/ADVANTAGE - For the selective sepn. of N2 from other gases, esp. natural gas.

Dwg.0/5

ABEQ US 5516745 A UPAB: 19960625

A composition comprising a hexacoordinate organometallic complex and a solvent having a solubility parameter of 20MPaone half, the organometallic complex consisting essentially of a **transition metal** selected from W, Fe, Co, and Mn and from one to six coordinating **ligands** capable of providing six coordinating atoms to the organometallic complex, at least one of the coordinating **ligands**

comprising bound nitrogen, the solvent being capable of dissolving the organometallic complex to 0.1M where the **ligands** are mono-, bi-, tetra- or pentadentate and are selected from the gp. consisting of halogens, hydrides carbon monoxide, amines, phosphines, phosphites, thiols and sulphides.
Dwg.0/5

ABEQ EP 546808 B UPAB: 19970516
A composition effective in absorbing nitrogen from hydrocarbons characterised in that the composition comprises a hexa-co-ordinate organometallic complex and a solvent selected from water, propylene carbonate, a glycol, and a glycolic oligomer, the organometallic complex consisting of a **transition metal** selected from Mo, W and Groups 7, 8 and 9 and at least one **ligand** capable of providing five co-ordinating atoms to the organometallic complex.
Dwg.0/5

L33 ANSWER 8 OF 14 MEDLINE
93308506 Document Number: 93308506. Constitutional, configurational and conformational analysis of **transition metal coordination complexes**. Leach A R. (Department of Chemistry, University of Southampton, U.K.) JOURNAL OF COMPUTER-AIDED MOLECULAR DESIGN, (1993 Apr) 7 (2) 225-40. Journal code: JCB. ISSN: 0920-654X. Pub. country: Netherlands. Language: English.

AB A computational approach to conformational analysis is applied to the study of **transition metal coordination complexes**. The method provides a means of rapidly exploring conformational space without any inherent reliance on energy calculations and is therefore applicable to a wide variety of systems. It has been incorporated into an algorithm which explores the constitutional, configurational and conformational degrees of freedom for a metal ion and a number of potential **ligands**. The program determines which of the possible **coordination complex** products could form stable conformations and can therefore be used to rationalise the products obtained from the **mixture**. The method is illustrated using two cases: the cobalt(III)-triethylenetetramine-glycine system and complexes of diindolopyridine derivatives.

L33 ANSWER 9 OF 14 CAPLUS COPYRIGHT 2000 ACS
1987:183495 Document No. 106:183495 Stabilities of bivalent metal complexes with biologically active 2-hydroxy-1,4-naphthoquinone monosemicarbazone (HNQS) in dioxane-water **mixtures**. Sharma, Rakesh Kumar; Sindhwani, Sharwan Kumar (Dep. Chem., Univ. Delhi, Delhi, 110007, India). Inorg. Chim. Acta, 135(3), 211-14 (English) 1987. CODEN: ICHAA3. ISSN: 0020-1693.

AB Equil. between 2-hydroxy-1,4-naphthoquinone monosemicarbazone and protons or bivalent metal ions were investigated potentiometrically at different ionic strengths and solvent compns. (dioxane:water). The method of Bjerrum and Calvin as modified by Irving and Rossotti was used to find the values of .lovin.n and pL. The stability consts. and the values of Smin = .chi.2 were calcd. The order of stability consts. is Cu > Pb > **Zn** > Ni > Co > Cd > Mn > Mg. The thermodn. parameters and **ligand** field stabilization energies were calcd. from the stability consts.

L33 ANSWER 10 OF 14 WPIDS COPYRIGHT 2000 DERWENT INFORMATION LTD
AN 1986-198608 [31] WPIDS
AB EP 189312 A UPAB: 19930922
O=contg. organic cpds. (I) are prepd. by oxidn. of an olefin (II) in the presence of a composite metallic complex catalyst. The catalyst components are: (a) a metallic complex (III) capable of forming an O2-**complex** by **coordination** with O2; (b) a metallic complex (IV) capable of forming an olefin **complex** by **coordination** with (II);

and (c) H2O. M = **transition metal** of Gps. I, IV-VII or the Fe gp. of Gp. VIII; X-= Cl-, Br-, I-, BF4-, PF4-, AcO-, SO42-; L = organic P cpd. or nitrile as **ligand** ; L' = one or more nitriles, organic F cpds. or organic P cpds. as **ligands**; M' = **transition metal** from the Pt. Gp. VIII metals, m, m', n, n' = constants to balance valencies; l, l' = no. of cordination.

ADVANTAGE - Use of the catalyst system allows the one-step oxidn. of olefins under milder reaction conditions in the presence of H2O. In the process the corresp. O-contg. cpds. are produced in a short time in high yield and high selectively. In add., the process is inexpensive.

0/5

ABEQ EP 189312 B UPAB: 19930922

A process for producing an oxygen-containing organic compound by oxidising an olefin in the presence of a metallic complex catalyst, which comrises as a catalyst component, a composite catalyst comprising a first metallic complex (MmXn asteriskeLl) capable of forming an oxygen **complex** by **coordination** thereof with oxygen, and a second metallic complex (M'mXn asteriskL'l) capable of forming an olefin **complex** by **coordination** thereof with said olefin, said M being a **transition metal** belonging to group 1, groups 1V-V11 of the iron group of group V111 of the Periodic Table, said X being at least one anion selected from Cl-, Br-, I-, BF4-, PF4-, CH3COO- and SO42-, said L as a **ligand** being an organic phosphorus compound or a nitrile, and L' as a **ligand** being at least one compound selected from nitriles, organic fluorine compounds and organic phosphorus compounds, said M' being a **transition metal** belonging to the platinum group of group V111 of the Periodic Table, said m, m', n and n' each being a constant to be determined by balance of the valences of said **transition metals** and said anion, and said l and l' each being a number of coordination, characterised in that the metallic complex catalyst further comprises as a catalyst component water which acts as an oxidising agent, and is present at an amount of 1.67 mol/l or more in a reaction solution.

ABEQ US 4806692 A UPAB: 19930922

In the prodn. of an O2-contg. organic cpd. by oxidn. of an olefin in the presence of a metallic complex catalyst, the improvement comprises using, as the catalyst, a composite catalyst comprising a metallic complex (MmXnLl) which forms an oxygen **complex** by **coordination** with oxygen, a metallic complex (M'm'Xn'Ll') which forms an olefin complex and water; adding an olefin to produce an olefin complex which is oxidised by water to form an oxygen-contg. cpd., M' and L', and adding an O2-contg. gas to form an oxygen-contg. complex. The oxygen-contg. complex is reacted with M' and L' to produce the metallic complex used in the oxidn. reaction.

In the formulae, M is at least one of Cu(1), Ag, Ti(3), Zr, Nb, Cr, Mo and W; X is Cl-, Br-, I-, BF4-, PF4-, CH3COO- and/or SO4(2-); L is a nitrile and/or organic P cpd.; L' is a nitrile, M' is a Pt gp. metal; m, m', n and n' are the number of atoms of the **transition metals** M and M' and anions X and X'; L and L' are the number of **ligands** L and L'.

ADVANTAGE - Oxygen-contg. organic cpds. are obtd. by oxidising olefins under milder conditions.

L33 ANSWER 11 OF 14 WPIDS COPYRIGHT 2000 DERWENT INFORMATION LTD

AN 1985-191883 [32] WPIDS

AB EP 150982 A UPAB: 19930925

Prodn. of acetone (I) is effected by oxidising propylene (II) with O2 in the presence of a composite catalyst comprising an O2-complexing metal complex of formula MmXnLp (IIIa) and a (II)-complexing metal complex of

formula M'xXyL'z (IIIb), where M = a **transition metal** of Gp. I or IV-VII or an Fe-group metal; X = an anion; L = an organophosphorus cpd.; M' = a Pt-group metal; L' = a nitrile, organic F cpd. or organophosphorus cpd.; m, n, x and y are nos. determined by the valences of M and M' and X; p and z are the no. of **ligands**.

ADVANTAGE - The process gives high yields (e.g. 48-97%) based on complexed O2) under mild conditions in a single reaction step.

0/2

ABEQ EP 150982 B UPAB: 19930925

A process for producing acetone by oxygen-oxidising propylene in the presence of a metal complex catalyst, which process comprises employing a composite catalyst contg. as the metal complex catalyst, a first complex (MmXn-Ll)capable of forming an oxygen **complex** by **coordination** of the first **complex** with oxygen and a second complex (M'm'Xn'-L'I'Ll) capable of forming a propylene **complex** by **coordination** of the second **complex** with propylene, wherein M is a **transition metal** selected from Cu and Ag of Gp. I, Ti and Zr of Gp.IV, V and Nb of Gp. V, Cr, Mo and W of Gp. VI, Mn of Gp. VII and Fe, Co and Ni of Gp. VIII of the Periodic Table, X is an anion selected from Cl-, Br-, I-, BF4-, PF6-, SO4(2)- and CH3COO-; L is an organic phosphorus cpd. as a **ligand** selected from phosphorous acid esters, phosphoric acid esters, phenylphosphinous acid esters, dimethylphosphinic acid esters, triethylphosphine, triphenylphosphine, triphenylphosphine oxide, dimethyl methylphosphonate, methyl dimethylphosphonate, hexamethylphosphoramide and one or more of alkoxy, alkyl and amide derivs. of phosphoric acid or phosphorous acid, M' is a **transition metal** selected from Pd, Ir and/or Pt; L' is a **ligand** selected from acetonitrile, propionitrile, benzonitrile, tolunitrile, phosphorous acid esters, phosphoric acid esters, phenylphosphinous acid esters, dimethylphosphinic acid esters, triethylphosphine, triphenylphosphine, triphenylphosphine oxide, dimethyl methylphosphonate, methyl dimethylphosphonate, fluorinated toluene, benzotrifluoride, hexamethylphosphoramide and one or more of alkoxy, alkyl and amide derivs. of phosphonic acid or phosphorous acid and m, m', n and n' are each a number determined by the valences of the above **transition metals** and the above anion, l and l' each the number of **ligands**, and m, m', n, n', l and l' are each an integer in the range of from 1-4.

ABEQ US 4605776 A UPAB: 19930925

Prodn. of acetone by oxygen-oxidising propylene in the presence of a metal complex catalyst which comprises using a composite catalyst. The composite catalyst contg. as the metal complex catalyst, a first complex (MmXnLl) capable of forming an oxygen **complex** by **coordination** of the **complex** with oxygen and (b) a second complex (M'm'Xn'L'l'Ll) capable of forming a propylene **complex** by **coordination** of the **complex** with propyelene.

M is a **transition metal** of gps. I, IV-VII, or the iron gp. of gp. VIII. X' is an anion. L is an organic phosphorus cpd. selected from triphenylphosphine, oxide, hexamethylphosphoramide, mono-, di- and triesters formed by the reaction of phosphoric acid with methanol and ethanol, dimethyl methylphosphonate methyl dimethylphosphinate, mono-, di- and triesters formed by the reaction of phosphorus acid with methanol and ethanol, phenylphosphinous acid esters, dimethylphosphonic acid esters, triethylphosphine and triphenyl phosphine M' is a platinum gp. **transition metal**. L' is a coordinating cpd. consisting of acetonitrile, propionitrile benzonitrile, tolunitrile, fluorinated toluene or benzotrifluoride. M,m' n and n' are each determined by valences of the above **transition metals** and the above anion.

L,l' are each the number of **ligands**.
USE/ADVANTAGE - Acetones are used as solvents commercially as well as
in pharmaceutical fields. They are used as synthetic raw materials for many intermediate prods. e.g. methyl isobutyl ketone etc.. The acetones are produced selectively and are obtd. in high yields under milder conditions and at a single stage.

L33 ANSWER 12 OF 14 BIOSIS COPYRIGHT 2000 BIOSIS
1984:280124 Document No.: BA78:16604. CYCLOPHANE PORPHYRINS AND THEIR METAL COMPLEXES BIOMIMETIC STUDY ON **RECEPTOR** SITE OF HEMO PROTEIN OXYGEN BINDING. OGOSHI H; SUGIMITO H; MIYAKE M; YOSHIDA Z-I. DEPARTMENT OF MATERIAL SCIENCE, TEHNOLOGICAL UNIVERSITY OF NAGAOKA, NAGAOKA, NI-IGATA, 949-54, JAPAN.. TETRAHEDRON, (1984) 40 (3), 579-592. CODEN: TETRAB. ISSN: 0040-4020. Language: English.
AB A new symmetric porphyrin, 7,8,17,18-tetraethyl-3,13-dimethylporphyrin-2,12-dipropionic acid and its derivatives were synthesized by the a,c-biladiene route. Condensation of the dipropionic acid with diamine, [H2N(CH2)NH2, n = 6,7,8,9,10,12 and 14], afforded the corresponding cyclophane porphyrins. The bridged groups were characterized by the 1H-NMR spectra of their **Zn** complexes. The spin state of the Fe(III) complexes of the cyclophane porphyrins was investigated by changing the size of the bridged chain or size of axial **ligand**. The cyclophane-porphyrinato(III) perchlorate complexes in a **mixture** of MeOH and CHCl3 with 4-benzylpyridine provide a model for methemoproteins. Steric constraint between an axial **ligand** and the bridge group, [-CH2CH2CONH(CH2)nNHCOCH2CH2] at the bridged face determines the ratio of the penta- and hexa-**coordinated** ferric **complexes**. The rate of O-binding of the Co(II) cyclophane porphyrins is markedly dependent on the size of the bridge chain. Removal of a solvent molecule or 6th axial **ligand** from the near proximity of the Co(II) complex probably increases the rate of O-binding.

L33 ANSWER 13 OF 14 CAPLUS COPYRIGHT 2000 ACS
1981:162633 Document No. 94:162633 Binary and ternary complexes of interest to environmental systems. Part VI. Interaction of **zinc**(II) with a **mixture** of **drugs**. Abbasi, Shahid Abbas (Sch. Biol. Sci., Bhopal Univ., Bhopal, India). Pol. J. Chem., 54(7-8), 1377-83 (English) 1980. CODEN: PJCHDQ.
AB In aq. solns. of **Zn**(II) and 5-nitrosalicylic acid (NSA), **Zn** failed to form mixed complex with 8-hydroxyquinoline-5-sulfonic acid-NSA and benzohydroxamic acid-NSA systems, although it formed binary complexes with each of the **ligands**. In equimolar mixts. of **Zn**(II), NSA, and 2,2'-bipyridyl, a 1:1 **Zn** (II)-2,2'-bipyridyl complex [41849-12-1] is formed and its formation is complete by pH 4. Above pH 4, NSA begins to **coordinate** with the **complex** to form a ternary complex [77070-01-0] of high stability. Computer-aided potentiometry was used in these studies. These systems may serve as models for the more complex metalloenzyme-**drug** in vivo interactions.

L33 ANSWER 14 OF 14 BIOSIS COPYRIGHT 2000 BIOSIS
1980:175439 Document No.: BA69:50435. OXYGEN DEPENDENT CLEAVAGE OF DNA BY THE 1 10 PHENANTHROLINE CUPROUS COMPLEX INHIBITION OF ESCHERICHIA-COLI DNA POLYMERASE I. SIGMAN D S; GRAHAM D R; D'AURORA V; STERN A M. DEP. BIOL. CHEM., SCH. MED., UNIV. CALIF., LOS ANGELES, CALIF. 90024, USA.. J BIOL CHEM, (1979 (RECD 1980)) 254 (24), 12269-12272. CODEN: JBCHA3. ISSN: 0021-9258. Language: English.
AB The 2:1 1,10-phenanthroline.cntdot.cuprous complex ((OP)2Cu+) inhibits the poly(dA-dT)-directed polymerization catalyzed by E. coli DNA polymerase I and other polymerases at concentrations of 0.1 .mu.M. This potent

inhibition was traced to an unexpectedly rapid cleavage of poly(dA-dT) by the **coordination complex** in an O2-dependent reaction that yields products which are effective inhibitors of the enzyme. For example, 0.8 .mu.M (OP)2Cu+ reduces by 80% the competence of 10 .mu.g/ml of poly(dA-dT) to serve as a primer/template for E. coli DNA polymerase I at pH 7.0 and 37.degree. C in a 2-min incubation under aerobic conditions.

The products must be inhibitory since quenching the reaction with 2,9-dimethyl-1,10-phenanthroline and adding supplementary poly(dA-dT) does not completely restore activity. Unambiguous evidence for a cleavage reaction is provided by analysis of incubation **mixtures** of DNA and (OP)2Cu+ using electrophoresis on agarose gels. Under aerobic conditions, the **coordination complex** causes the depolymerization of poly(dA-dT) and relaxation of closed SV-40 supercoiled DNA to nicked circles. A central role for O2 is demanded by the sharp dependence of the cleavage reaction on the concentration of O2 and the blockage of the reaction by the addition of catalase to incubation **mixtures** containing O2 and thiol. Since the reaction of (OP)2Cu+ with DNA resembles the cleavage reaction of the antitumor **drugs** bleomycin and neocarzinostatin, the cytotoxic properties of this simple **coordination complex** may be of interest. The rapid cleavage reaction reported here must be considered before 1,10-phenanthroline inhibition is interpreted in terms of coordination to the tightly bound **Zn** ion in DNA and RNA polymerases.

L35 ANSWER 1 OF 24 WPIDS COPYRIGHT 2000 DERWENT INFORMATION LTD
AN 2000-156693 [14] WPIDS
AB JP2000017010 A UPAB: 20000323
NOVELTY - A conjugated diene compound is polymerized using catalyst obtained from ionic compound of (A) metallocene type complex of V group **transition metal** compound, (B) non-coordinating anion and cation, (C) organo aluminum compound and (D) water. The organo aluminum compound and water are mixed before adding into catalyst **mixture** containing A,B and C.

USE - For conjugated diene polymer preparation such as polybutadiene.

ADVANTAGE - The micro structure of conjugated diene polymer is controlled. Polymerization activity is enhanced.

Dwg.0/0

L35 ANSWER 2 OF 24 WPIDS COPYRIGHT 2000 DERWENT INFORMATION LTD
AN 2000-053228 [04] WPIDS
AB WO 9959811 A UPAB: 20000124
NOVELTY - Ultradisperse nanoparticles of hydrated oxide for use in structuring biological media in a structure comprising (a) particle; (b) biological tissue and (c) surrounding media, the structured biological media comprising three-sided biological system.

DETAILED DESCRIPTION - An INDEPENDENT CLAIM is also included for method of modifying surface of ultradisperse nanoparticles of hydrated oxides by partial methylation.

ACTIVITY - Bactericidal; cosmetic; dental.

USE - Used in structuring biological media (claimed). Used in toothpastes, to treat inflamed gum tissue, for direct delivery of fluoride to tooth enamel, in chewing gums for use as dentifrice, in medicinal, cosmetic, hygiene, agricultural, water-treatment and disinfection applications, and in the food industry (all claimed). Used in skin creams.

Used in applications requiring radioactivity to reduce level of radioactivity needed thus reducing exposure. Used as safe and effective preservatives and stabilizers. Used to provide slow-release mechanisms. Used to increase sensitivity to antibiotic treatment, enabling more effective use of antibiotics at lower doses. Bind toxins released by infection to give general cleansing effect and reducing need to activate immune system giving body more strength to heal itself in shorter time. Used as hygienic body was h for all body cavities including surgical cavities. Used as exfolient cream to peel and absorb dead skin, to extract oil from skin pores without damage. Used in agriculture as biological exterminants. Used to deliver calcium fluoride to treat scars and keloids, magnesium to treat pruritis senilis, barium carbonate to treat cuprosis, sulfur and silicon dioxide to treat acne vulgaris and calcium sulfide to dissolve its scar tissue, silver nitrate as local disinfectant and to aid blood clotting with cauterizing effect on tissues for diabetic patients in whom healing process is especially slow, and **zinc** to treat balding caused by alopecia. Patients were treated with antibiotic alone or in presence of ultradisperse particles. Results for the following antibiotics alone or with particles, respectively, were as follows: penicillin 20 and 33; ampicillin 60 and 67; streptomycin 60 and 100; gentamycin 80 and 100; tetracycline 40 and 67; levomycitin 40 and 67; erythromycin 40 and 100 and kanamycin 80 and 100. The results show that, in all cases, sensitivity to antibiotics was boosted by use of

ultradisperse particles.

ADVANTAGE - Surface structure of ultradisperse particles may be altered to allow predetermined interactions to take place in biological media. Sequential and/or simultaneous actions may be performed by 'multi-action' particles. In skin creams, when skin is dry, oil is attracted to skin, and when skin needs water, water is attracted to skin, thus providing skin with treatment that it needs. Provide broad-spectrum bactericidal protection at lower concentrations than conventional preservatives and stabilizers. Particles reduce significantly amount of silica needed to function as preservative. Able to deal with different states in selective manner.

Dwg.0/16

L35 ANSWER 3 OF 24 WPIDS COPYRIGHT 2000 DERWENT INFORMATION LTD

AN 2000-063561 [06] WPIDS

AB DE 19825713 A UPAB: 20000203

NOVELTY - A process for the production of polymers of vinyl aromatic compounds in a dispersion in the presence of a dispersing agent and a catalyst prepared from:

(A) a **transition metal** complex of a group II-VIII element;

(B) a cationic agent; and optionally

(C) aluminum compound

is characterized by the addition of a lubricant.

USE - The process is useful for the preparation of vinyl aromatic polymers for the production of fibers, film and molded articles.

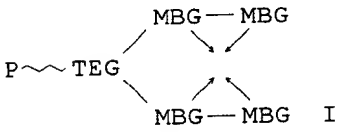
ADVANTAGE - The process utilizes a low viscosity reaction **mixture** and has an improved yield and productivity. The resulting syndiotactic polymer product has a high mol. wt.

Dwg.0/0

L35 ANSWER 4 OF 24 CAPLUS COPYRIGHT 2000 ACS

1998:197471 Document No. 128:265374 **Combinatorial** approach for generating novel **coordination complexes**. Jacobsen, Eric N.; Francis, Matthew B.; Finney, Nathaniel S. (President and Fellows of Harvard College, USA; Jacobsen, Eric N.; Francis, Matthew B.; Finney, Nathaniel S.). PCT Int. Appl. WO 9812156 A1 19980326, 89 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1997-US16740 19970919. PRIORITY: US 1996-26432 19960920.

GI



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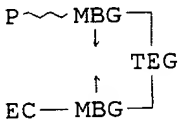

II

AB The present invention provides methods and compns., i.e. synthetic **libraries** of binding moieties, for identifying compds. which bind to a metal atom or to non-metal ions, e.g., cationic or anionic mols. Thus, **combinatorial libraries**, e.g. I and II (P = TentaGel S amino resin polymer support; TEG = turn element group, i.e. di- or trifunctional cyclic amino alc. or cyclic amino acid; MBG = metal binding group, i.e. amino acid residue; EC = end capping group, i.e. acyl residue) were prepd. and examd. for their ability to coordinate **transition metal** ions. Thus, a 12,000 member

combinatorial library P-NHCO(CH2)5NH-A-B-C-D [III; P-NH2 = TentaGel S amino resin polymer; A (position 1) = L- or D-Asp(OCMe3), L- or D-Ser(CMe3), L- or D-Met, L- or D-Tyr(CMe3), L- or D-phenylglycine, His(CPh3), Gly; C (position 2) = L-Asp(OCMe3), L-Ser(CMe3), L-Tyr(CMe3), L-His(CPh3), L-Met, L-Trp, Gly, L-phenylglycine, 4-piperidinecarboxylic acid; B (turn element) = 1-amino-2-carbonyloxycyclopentane stereoisomers, 1-amino-2-carbonyloxycyclohexane stereoisomers, 1-amino-2-carbonyloxyindane stereoisomers, L-Pro, D-pipecolinic acid; D (end cap) = RCO, tosyl, pyroglutamic acid, R = Me, CMe3, 1-naphthyl, CH2CO2Me, 2-pyridyl, 3,4-methylenedioxyphenyl, PhNH] was prepd. using std. solid-phase peptide coupling techniques. **Library** III was tested for Ni2+ binding affinity by treatment with 2.5 .times. 10-4 M Ni(OAc)2 in MeOH followed by soln. of dimethylglyoxime in MeOH to form a reddish-pink ppt. trapped in the polymer matrix of about 6 of the 24,000 beads. Tag photolysis and anal. allowed the identification of the individual nickel-binding **library** members.

L35 ANSWER 5 OF 24 WPIDS COPYRIGHT 2000 DERWENT INFORMATION LTD
AN 1998-348118 [30] WPIDS
AB WO 9822413 A UPAB: 19980730
A halogen exchange process comprises heating a **mixture** of at least one finely divided alkali metal fluoride (AMF), at least one haloaromatic compound (I) (containing at least one halo other than F on an aromatic ring) and an aminophosphonium catalyst (II) so that the halo of (I) is replaced by fluoro. Also claimed are processes involving a preferred halogen exchange as above plus further conversion(s) of the product, typically consisting of: (i) heating a **mixture** of KF, RbF or CsF, C6FnX6-n (I') (X = Cl or Br; n = 0-4) and (II); (ii) recovering obtained chloro-pentafluorobenzene (C5FB) or bromo-pentafluorobenzene (B5FB); (iii) converting the product into a pentafluorophenyl Grignard reagent or alkali metal compounds; (iv) optionally converting the product into a pentafluorophenyl boron compound by reaction with a boron halide or its etherate; and (v) optionally contacting the product with a metallocene of formula LMX2 (III) to form a catalyst having a limiting charge separated structure of formula LMX+.XA- (IV). L = derivative of a delocalised pi -bonded group imparting a constrained geometry to the metal active site and containing up to 50 non-H atoms; M = group 4 metal; X = H or a hydrocarbyl, silyl or germyl group having up to 20 C, Si or Ge atoms; A = anion formed from the product of (iv). In a variant on the process, step (i) involves more specific conditions and step (v) more generally involves converting the product into a **coordination complex** containing a tetra-(pentaphenylborate) anion; and, if the complexing component is a cyclopentadienyl compound of a Group IV **transition metal**, the process optionally includes adding further components to give an active catalyst.

USE - The process is useful for producing polyfluorinated aromatic compounds, especially starting materials to be converted into tetrakis-(pentafluorophenyl)-borate components of polymerisation catalysts. The process is especially for polyfluorination of hexachlorobenzene (6CB), pentachlorofluorobenzene, tetrachlorodifluorobenzene, trichlorotrifluorobenzene (3C3FB) and dichlorotetrafluorobenzene (2C4FB).

ADVANTAGE - A wide variety of fluorinated aromatic compounds can be produced efficiently and cheaply under relatively mild reaction conditions on a large scale with increased yields. The starting material (I) may contain or be free of activating groups.

Dwg.0/1

L35 ANSWER 6 OF 24 WPIDS COPYRIGHT 2000 DERWENT INFORMATION LTD
AN 1998-388814 [34] WPIDS
AB DE 19700305 A UPAB: 19980826

A process for the production of polymers of vinyl-aromatic compounds (I) comprises polymerisation of (I) in a dispersion in presence of a dispersant (II) and a catalyst derived from (A) a Sub-Group II-VIII **transition metal** complex, (B) a cation-forming agent and optionally (C) an aluminium compound.

Dispersant (II) is a block copolymer with a diene block (B) and block(s) (S) of a copolymer of vinylaromatic monomer and 1,1-diphenylethylene (DPE) or substituted derivatives thereof with 1-22C alkyl groups on the aromatic rings.

Preferably, block B is based on polybutadiene or polyisoprene, and may be unhydrogenated or partly or completely hydrogenated, and block S is a copolymer of styrene and DPE.

The amount of (II) used is 0.1-10 wt.% based on (I), and the dispersion medium consists of aliphatic hydrocarbons.

A branching comonomer (IA) with at least two vinylaromatic residues may also be used, in a mol ratio of (I):(IA) = (107:1)- (10:1).

Catalyst component (A) is a metallocene complex of formula (III), in which R7-R11 = H, 1-10C alkyl, 5- to 7-membered cycloalkyl (optionally substituted with 1-6C alkyl), 6-15C aryl or aralkyl (or two adjacent groups may form 4-15C cyclic groups), or Si(R12)3; R12 = 1-10C alkyl, 6-15C aryl or 3-10C cycloalkyl; M = a Sub-Group III-VI metal or a metal of the lanthanide series; Z1-Z5 = H, halogen, 1-10C alkyl or alkoxy, or 6-15C aryl or aryloxy; z1-z5 = 0, 1, 2, 3, 4 or 5; the sum of z1-z5 = the valency of M minus 1.

Component (B) is an aluminoxane of formula (IV) or (V), in which R13 = 1-4C alkyl and m = 5-30, or a **coordination complex** selected from strong neutral Lewis acids, ionic compounds with Lewis acid cations and ionic compounds with Bronsted acid cations.

USE - The polymers obtained are used for the production of fibres, films and mouldings.

ADVANTAGE - Enables the production of syndiotactic vinylaromatic polymers with a low-viscosity reaction **mixture** in a conventional stirred reactor, and without the other disadvantage of prior art processes (coating of reactor with crystallised polymer, special equipment such as fluid bed reactors or extruders, high pressure, etc.)

Dwg.0/0

L35 ANSWER 7 OF 24 WPIDS COPYRIGHT 2000 DERWENT INFORMATION LTD

AN 1997-244352 [22] WPIDS

CR 1995-216788 [28]; 1995-216807 [28]; 1996-412100 [41]; 1997-258244 [23]; 1997-525237 [46]; 1998-041332 [04]; 1998-052015 [05]; 1998-075891 [05]; 1998-177930 [14]; 1998-260043 [22]; 1998-413120 [35]

AB US 5622682 A UPAB: 19980904

The recovery of halocarbon compounds from effluent gas streams containing 0.1-5 wt.% of halocarbon (based on the total weight of the effluent gas stream) chosen from perfluorocarbons, fluorinated hydrocarbons and chlorofluorocarbons and/or sulphur hexafluoride; and acidic gas component(s), comprises: (a) contacting the effluent gas stream with a scavenger composition chosen from goethite, copper oxide, copper oxide/ **zinc** oxide **mixtures**, copper sulphate, calcium oxide or lithium hydroxide; and a synthetic metallic scavenger comprising a caustic liquid medium containing a 3-dimensional **complex** of several metal **coordination** atoms each coordinated with at least 2 different oxomeric moieties (the oxomeric moieties bridge between the metal atoms) selected from carbonate, sulphite, carboxylate and silicate; (b) removing the acidic gas component(s) from the effluent gas stream to obtain a first effluent gas **mixture** containing the halocarbon; (c) contacting the first effluent gas **mixture** with an adsorbent for the halocarbon component of the first effluent gas **mixture** to yield a second effluent gas; and (d) recovering the adsorbed halocarbon

from the adsorbent. In (c), contact with the adsorbent is carried out in at least 2 adsorbent beds by pressure swing adsorption.

USE - The process is useful in semiconductor etching, chemical vapour deposition (CVD), silicon processing and cleaning applications, using especially perfluoroethene, perfluoroethane, trifluoromethane and carbon tetrachloride (claimed). The corrosive by-product acidic gases removed in the process are, e.g., hydrogen fluoride, boron trifluoride, hydrogen chloride, chlorine and silicon tetra:fluoride (claimed) which are hazardous to personnel and recycling equipment.

ADVANTAGE - The process can be used with effluent gas which intermittently contain halocarbons (claimed). The scavengers are stable under storage at room temperature and exposure to air or moisture does not affect their effectiveness. A clean, concentrated stream of recovered halogenated compound, suitable for recycling is obtained (claimed). Improved volumetric efficiency is obtained, compared with prior art scrubber materials.

Dwg.0/4

L35 ANSWER 12 OF 24 EMBASE COPYRIGHT 2000 ELSEVIER SCI. B.V.

90188934 EMBASE Document No.: 1990188934. Asymmetric synthesis of .alpha.-amino-.beta.-hydroxy acids using a chiral pyridoxal-like pyridinophane-**zinc** complex as an enzyme mimic; scope and limitation. Ando M.; Watanabe J.; Kuzuhara H.. Institute of Physical and Chemical Research, Wako-shi, Saitama 351-01, Japan. Bulletin of the Chemical Society of Japan 63/1 (88-90) 1990.

ISSN: 0009-2673. CODEN: BCSJA8. Pub. Country: Japan. Language: English. Summary Language: English.

AB A chelate complex (4) with high homogeneity was precipitated upon stirring a **mixture** of **zinc**(II) ion and a Schiff base produced from glycine and (R)- or (S)-15-formyl-14-hydroxy-2,8-dithia[9](2,5)pyridinophane, chiral pyridoxal-like pyridinophane. A four-**coordinated zinc** chelate **complex** was newly proposed as the structure of 4. Aldol condensations between 4 and several aldehydes were attempted at pH 10.0. Only small linear chain aldehydes, such as acetaldehyde and propionaldehyde, could react with 4 under these conditions to give the corresponding .alpha.-amino-.beta.-hydroxy acid in the range of 27-77% enantiomeric excess.